MATHEMATICAL METHODS OF QUANTUM MECHANICS SUMMARY

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Abstract.

Contents

Postulates of Quantum Mechanics

Quantum mechanical system	separable Hilbert space $\mathscr{H}$
State	$\psi \in \mathscr{H}, \|\psi\| = 1$
Observables	Self-adjoint operators on $\mathscr{H}$
Expected Value of an observable A in the state ψ	$\langle \psi, A\psi \rangle$
Variance of an observable A in the state ψ	$\Delta A_\psi := \langle \psi, A^2\psi \rangle - \langle \psi, A\psi \rangle^2$

Lemma 1.1 (Heisenberg Uncertainity Principle). *Let A and B two self-adjoint operators on a Hilbert space $\mathscr{H}$. Then for any state ψ*

$$\Delta A_\psi \Delta B_\psi \geq \frac{1}{4} |\langle \psi, [A, B]\psi \rangle|^2 .$$

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Unbounded Operators

Definition 1.1 (Linear Operator). *Let $\mathcal{H}$ be a Hilbert space. A **(linear) operator on $\mathcal{H}$** is simply a linear map $A : D(A) \to \mathcal{H}$, where $D(A)$ is a linear subspace of $\mathcal{H}$.*

Examples 1.1.

(a) (***Multiplication operator***) Let $\mathcal{H} := L^2(\mathbb{R})$ and consider $\hat{x} : D(\hat{x}) \to L^2(\mathbb{R})$ defined by $(\hat{x}\psi)(x) := x\psi(x)$ (or $(\hat{f}\psi)(x) := f(x)\psi(x)$ for any complex valued measurable function f).

(b) (***Differential operator***) Let $\mathcal{H} := L^2(\mathbb{R})$ and consider $\nabla : C^\infty(\mathbb{R}) \to L^2(\mathbb{R})$.

Definition 1.2 (Closed Operator). *An operator A on $\mathcal{H}$ is said to be **closed**, iff Γ_A is closed in $\mathcal{H} \times \mathcal{H}$.*

Definition 1.3 (Closable Operator). *An operator A on $\mathcal{H}$ is said to be **closable**, iff $\overline{\Gamma}_A$ is a linear graph, i.e. $(0, y) \in \overline{\Gamma}_A$ implies $y = 0$. The corresponding operator associated to $\overline{\Gamma}_A$ is denoted by $\overline{A}$ and called the **closure** of A. Clearly $A \subseteq \overline{A}$.*

Definition 1.4 (Adjoint). *Let A be a densly defined operator on $\mathcal{H}$. Set*

$$D(A^*) := \{\psi \in \mathcal{H} : \exists \eta \in \mathcal{H} \text{ s.t. } \forall \varphi \in D(A)\ \langle A\varphi, \psi\rangle = \langle \varphi, \eta\rangle\},$$

*and $A^*\psi := \eta$. The operator A^* is called the **adjoint** of A.*

Theorem 1.1. *Let A be a densly defined operator on $\mathcal{H}$. Then:*

(a) A^* is closed.

(b) A is closable if and only if $D(A^*)$ is dense.

(c) If A is closable, then $(\overline{A})^* = A^*$.

Definition 1.5 (Symmetric Operator). *A densly defined operator A is said to be **symmetric**, iff $A \subseteq A^*$.*

Definition 1.6 (Self-adjoint Operator). *A densly defined operator is said to be **self-adjoint**, iff $A = A^*$.*

Example 1.1. Let A_f denote the multiplication operator. Then $A_f^* = A_{\overline{f}}$.

Definition 1.7 (Essentially Self-adjoint Operator). *A symmetric operator A is said to be **essentially self-adjoint**, iff $\overline{A}$ is self-adjoint.*

Example 1.2. Let $\mathcal{H} := L^2[0, 2\pi]$ and consider the operator A defined by $A := -i\frac{d}{dx}$ with $D(A) := \{\psi \in C^1[0, 2\pi] : \psi(0) = \psi(2\pi)\}$.

Theorem 1.2. *Let A be a symmetric operator. Then the following statements are equivalent:*

(a) A is self-adjoint.

(b) A is closed and $\ker(A^* \pm i) = \{0\}$.

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(c) $\mathrm{im}(A \pm i) = \mathcal{H}$.

Lemma 1.2 (Weyl Lemma). *Let A be a closed densly defined operator such that there exists a sequence $(\psi_n)_{n\in\omega}$ in $D(A)$ with $\|\psi_n\| = 1$ for all $n \in \omega$ and $\|(A-z)\psi_n\| \to 0$ for some $z \in \mathbb{C}$. Then $z \in \sigma(A)$ (the sequence $(\psi_n)_{n\in\omega}$ is called a* ***Weyl sequence****).*

Theorem 1.3. *Let A be a symmetric closed operator. Then A is self-adjoint if and only if $\sigma(A) \subseteq \mathbb{R}$.*

The Spectral Theorem

Projection Valued Measures.

Definition 1.8 (Projection Valued Measure). *Let $\mathcal{H}$ be a Hilbert space. A function*

$$P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$$

is said to be a ***projection valued measure****, iff*
(i) For all $\Omega \in \mathcal{B}(\mathbb{R})$, $P(\Omega)$ is an orthogonal projection, i.e. $P(\Omega)^2 = P(\Omega) = P(\Omega)^*$.
(ii) $P(\mathbb{R}) = \mathrm{id}_{\mathcal{H}}$.
(iii) If $(\Omega_n)_{n\in\omega}$ is a sequence of pairwise disjoint elements of $\mathcal{B}(\mathbb{R})$, then

$$P(\Omega)\psi = \sum_{n\in\omega} P(\Omega_n)\psi,$$

for all $\psi \in \mathcal{H}$.

Definition 1.9 (Resolution of the Identity). *Let $\mathcal{H}$ be a Hilbert space and P a projection valued measure. The function $p : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ defined by*

$$p(\lambda) := P\left(-\infty, \lambda\right],$$

is called the ***resolution of the identity associated to a projection valued measure****.*

Functional Calculus. Let $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ be a projection valued measure. Then for any simple function $f := \sum_{k=1}^n \alpha_k \chi_{\Omega_k}$ we define

$$P(f) := \int_{\mathbb{R}} f(\lambda) dp(\lambda) := \sum_{k=1}^n \alpha_k P(\Omega_k).$$

Since the simple functions are dense in the space of *bounded Borel functions* (with respect to $\|\cdot\|_\infty$) $\mathcal{M}_b$, we can extend above definition to $\mathcal{M}_b$. Actually, this defines a C^*-algebra homomorphism.
Consider now f just a Borel function. Then we get an operator $P(f) : D(P(f)) \to \mathcal{H}$ where

$$D(P(f)) := \left\{\psi \in \mathcal{H} : f \in L^2(\mathbb{R}, d\mu_\psi)\right\},$$

defined by

$$P(f)\psi := \lim_{n\to\infty} P(f_n)\psi,$$

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where $f_n := f\chi_{|f|\le n}$. We write

$$P(f) = \int_{\mathbb{R}} f(\lambda) dp(\lambda).$$

Existence. Existence is guaranteed by *Herglotz* or *Nevanlinna* functions.

Theorem 1.4 (Spectral Theorem). *Let A be a self-adjoint operator. Then there exists a unique projection valued measure P^A such that $D(A) = \{\psi \in \mathcal{H} : \int |\lambda|^2 \, d\mu_\psi^A(\lambda) < \infty\}$ and*

$$A = \int \lambda dp^A(\lambda).$$

Theorem 1.5. *Let A be a self-adjoint operator with projection valued measure P^A. Then*

$$\sigma(A) = \{\lambda \in \mathbb{R} : \forall \varepsilon > 0 \; P^A(\lambda - \varepsilon, \lambda + \varepsilon) \neq 0)\}.$$

Definition 1.10 (Spectral Basis). *Let A be a self-adjoint operator. A family $(\psi_\iota)_{\iota\in I}$ in $\mathcal{H}$ is said to be a* ***spectral basis*** *of $\mathcal{H}$, iff $\mathcal{H}_{\psi_i} \perp \mathcal{H}_{\psi_j}$ for all $i \neq j$, where*

$$H_{\psi_i} := \{f(A)\psi_i \in \mathcal{H} : f \in L^2(\mathbb{R}, d\mu_{\psi_i})\},$$

and $\mathcal{H} = \bigoplus_{\iota\in I} \mathcal{H}_{\psi_\iota}$.

Now for any self-adjoint operator there exists a at most countable spectral basis $(\psi_\iota)_{\iota\in I}$ and a unitary operator $U : \mathcal{H} \to \bigoplus_{\iota\in I} L^2(\mathbb{R}, d\mu_{\psi_\iota})$ such that $Uf(A)U^* = f$, where f acts as a multiplication operator on each coordinate. Thus *any self-adjoint operator is unitarly equivalent to a multiplication operator*.
Moreover, for any Borel measure μ we have a decomposition

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{\mathrm{ac}}) \oplus L^2(\mathbb{R}, d\mu_{\mathrm{pp}}) \oplus L^2(\mathbb{R}, d\mu_{\mathrm{sc}}).$$

The Schrödinger Equation.

Theorem 1.6. *Let $\mathcal{H}$ be a Hilbert space and $H : D(H) \to \mathcal{H}$ be self adjoint. Moreover, set $U(t) := \exp(-iHt)$ for $t \in \mathbb{R}$. Then:*
(a) *$U(t)$ is a strongly continuous one parameter unitary group.*
(b) *The limit*

$$\lim_{t\to 0} \frac{U(t) - 1}{t}\psi$$

exists if and only if $\psi \in D(H)$. Then

$$\lim_{t\to 0} \frac{U(t) - 1}{t}\psi = -iH\psi.$$

(c) *$U(t)D(H) = D(H)$ and $[U(t), H] = 0$ on $D(H)$.*

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(d) Let $\psi_0 \in D(H)$. Then $U(t)\psi_0$ uniquely solves the initial value problem

$$\begin{cases} i\partial_t \psi(t) = H\psi(t) \\ \psi(0) = \psi_0, \end{cases} \tag{1}$$

*called the **Schrödinger equation**.*